北京大学量子材料科学中心

International Center for Quantum Materials, PKU

Seminar

Energy Level Alignment and Atomic-Scale Interactions at Interfaces from First Principles

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地点：北京大学物理楼，西563会议室

Abstract

Interfaces are everywhere around us. The alignment of energy levels at interfaces in devices determines the device contact resistance, while the atomic-scale interactions at interfaces influence macroscopic experimental observables. In this talk, I will describe how my group has used first principles calculations to study a variety of interfacial phenomena in organic-inorganic heterostructures as well as 2D material systems. Energy level alignment (ELA) is an important but challenging problem from both theoretical and experimental points of view. Theoretically, it is widely known that quantitative predictions of ELA require methods beyond standard density functional theory, the work-horse of first principles calculations. ELA can be predicted quantiatively using many-body perturbation theory in the GW approximation, but GW calculations are computationally very expensive for large interface systems. In this work, we develop approaches to predict ELA at the GW level using computationally tractable methods. Using a simple but powerful approach, called XAF-GW [1], we can perform GW calculations of large interface systems without strong covalent bonds. We show analytically that the approach works for hybridized systems up to first order in the overlap matrices, and validate our approach using bilayer black phorphorus, where interface hybridization takes place. XAF-GW allows us to perform GW calculations of PTCDA layers on Au and Ag substrates, as well as on graphite-supported WSe_2 substrates. We further propose simple back-of-the-envelope estimates of the ELA for small physisorbed molecules on any substrate, and study the non-local screening effects of 2D materials [2]. The physics of screening at hybridized organic-metal interfaces is also investigated [3]. Besides ELA, atomic-scale interactions at interfaces can also lead to interesting experimentally observable properties, even in 2D layered materials where interfacial interactions are thought to be weak. We predict an electric-field induced Dirac cone in black phosphorus thin films which we show arises from quantum confinement and anisotropic interlayer interactions [4], that are unusually large in this material. The unusually large interlayer interactions were deduced from the computed frequencies of interlayer breathing modes [5], that were confirmed in experiment. Such interlayer interactions also result in experimentally observable stacking sequence dependent frequency trends in the interlayer shear modes for 2D materials in general [6]. Surface effects resulting from the removal of interlayer interactions are also responsible for anomalous frequency trends in transition metal dichalcogenide systems [7].

[1] *Journal of Chemical Theory and Computation*, 15, 3824 (2019)
[2] *2D Materials*, 6, 035036 (2019)
[3] *J Phys Chem C*, 121, 13125 (2017)
[4] *Scientific Reports* 5, 11699 (2015)
[5] *Nano Letters*, 15, 3931 (2015)
[6] *Scientific Reports* 5, 14565 (2015), *Advanced Materials*, 27, 4502 (2015)
[7] *Physical Review B*, 88, 075320 (2013)

About the speaker

Su Ying Quek is an Assistant Professor in the National University of Singapore (NUS). She joined NUS in 2013, from the Institute of High Performance Computing in Singapore, where she was a Senior Scientist. She was awarded the National Research Foundation Fellowship in 2013, as well as the Institute of Physics Nanotechnology Physics Medal and Prize in 2016.

Su Ying has a BA Honors (1st class) degree in Mathematics from the University of Cambridge (2000) and a PhD in Applied Physics from Harvard University (2006). She was an exchange student in University of California Berkeley from 2005 to 2006, and was a post-doc in Lawrence Berkeley National Laboratory from 2006 to 2010. She is actively involved in research activities as well as the supervision of graduate students and undergraduate teaching. Her group has worked extensively on experimentally relevant problems, explaining and making predictions on macroscopic observables from first principles quantum mechanical properties. They are also actively involved in methodological developments to incorporate many-electron effects on quasiparticle and optical spectra into more computationally tractable models. Su Ying has 60 publications and a h-index of 30.